Accelerating Deployment of Clean and Secure Energy Technologies from Coal

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Clean and Secure Energy from Coal: Budget

1 Oct 2008 - 30 Aug 2013

- Oxy-Coal 4,092,525
- Gasification 2,697,184
- Chemical Looping Combustion 1,741,336
- Underground Coal Thermal Treatment . 731,616
- Sequestration 198,176
- Mercury 51,168
- Sequestration Policy 605,419

Total 12,382,153

total oxy-coal:
DOE: 3,274,020
cost share:
818,505

to date:
1,435,981

Clean and Secure Energy from Coal: Participants

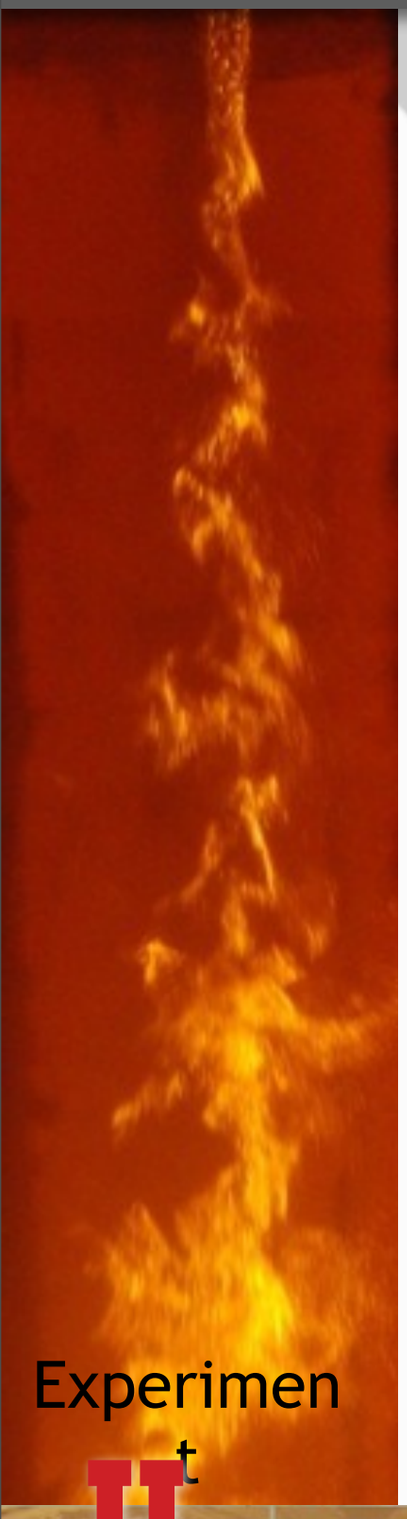
- Faculty:
  - Lincoln Davies, Milind Deo, Eric Eddings, Ted Eyring, JoAnn Lighty, Ron Pugmire, Arnold Reitze, Terry Ring, Adel Sarofim, Philip Smith, James Sutherland, Jeremy Thornock, Jost Wendt, Kevin Whitty, Larry Baxter (BYU), Tom Fletcher (BYU)
- Research staff and postdoctoral fellows:
  - Kerry Kelly, Gabor Konya, Michal Hradisky, Ryan Okerlund, Dana Overacker, Ignacio Preciado, Heather Tanana, Kirsten Uchitel, David Wagner, Hongzhi Zhang
- Students:
  - Milo Alvarez, Richard Baracki, Chris Clayton, Ben Coates, Keith Gneishin, Issac Hunsaker, Ben Isacc, Junlu Jia, Rob Krumm, Prashanth Mandalaparty, Will Morris, Julien Pedel, Naveen Puntai, Dadmier Rezaei, Charles Reid, Asad Sahir, Randy Schurtz (BYU), Pal Toth, Travis Waind, David Ray Wagner, Li Yang
- Administrative staff:
  - Andrew Morgenegg, Jeri Schryver, Adam Taylor, Catrina Wilson

Clean and Secure Energy from Coal: Objectives

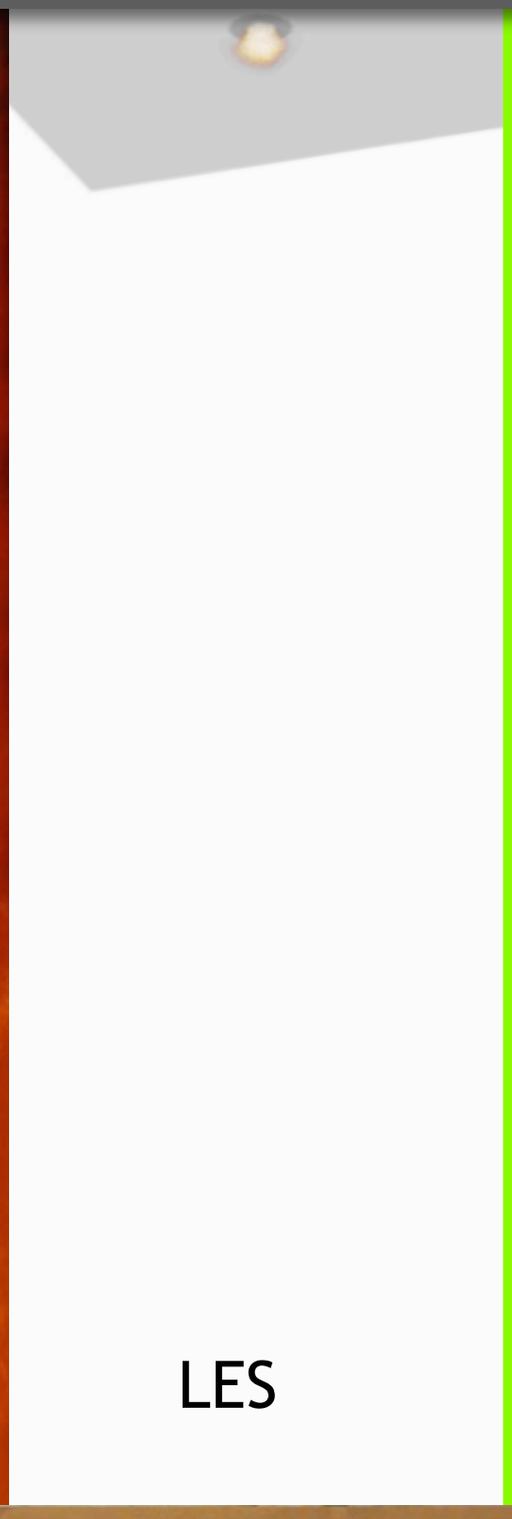
- **Goal:** Accelerate technology deployment through tightly coupled simulations and experiments for oxy-coal combustion to predict performance with quantified uncertainty.

- **Success Criteria** include:
  - engaging industry to deploy the simulation tools and to accelerate technology deployment.
  - quantifying uncertainty for selected quantities of interest and obtaining consistency between the simulation and experimental measures.

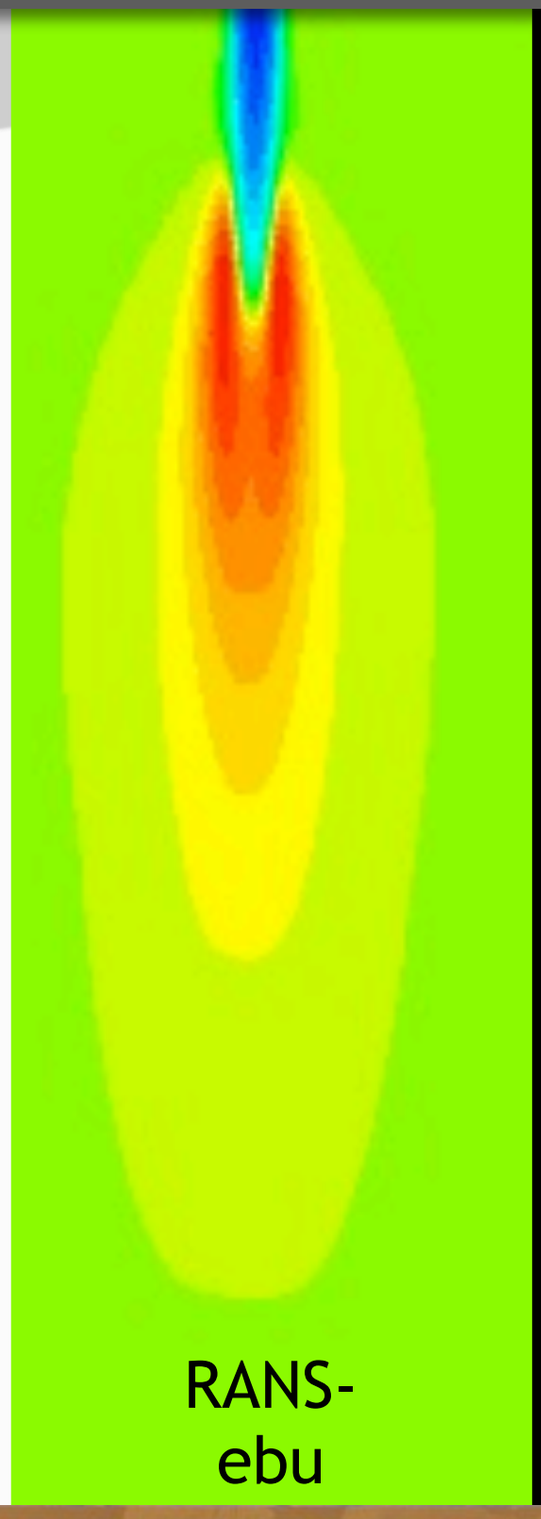
Accelerate Deployment: HPC (oxy-coal)



Experiment



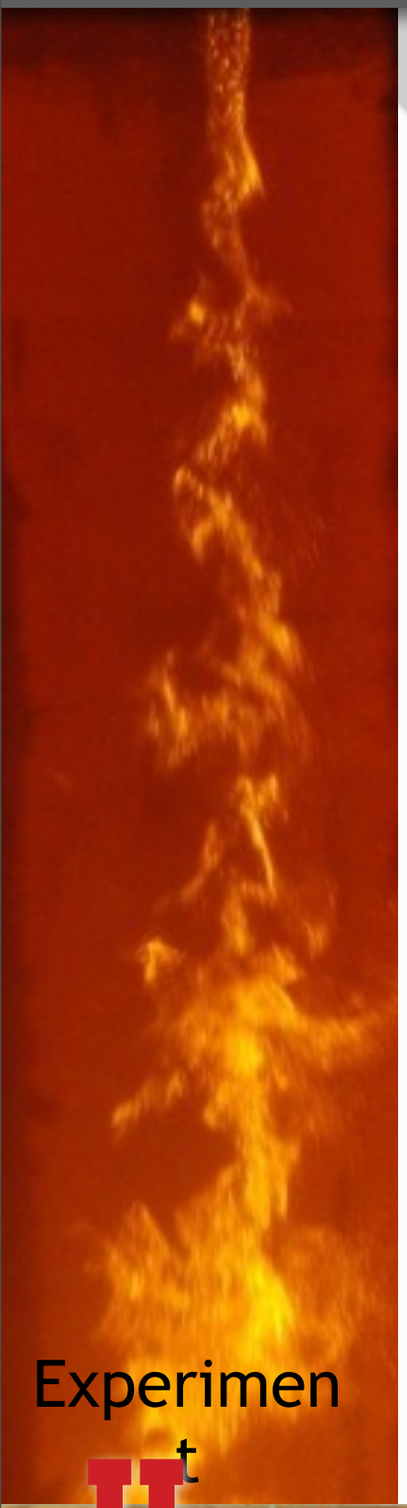
LES

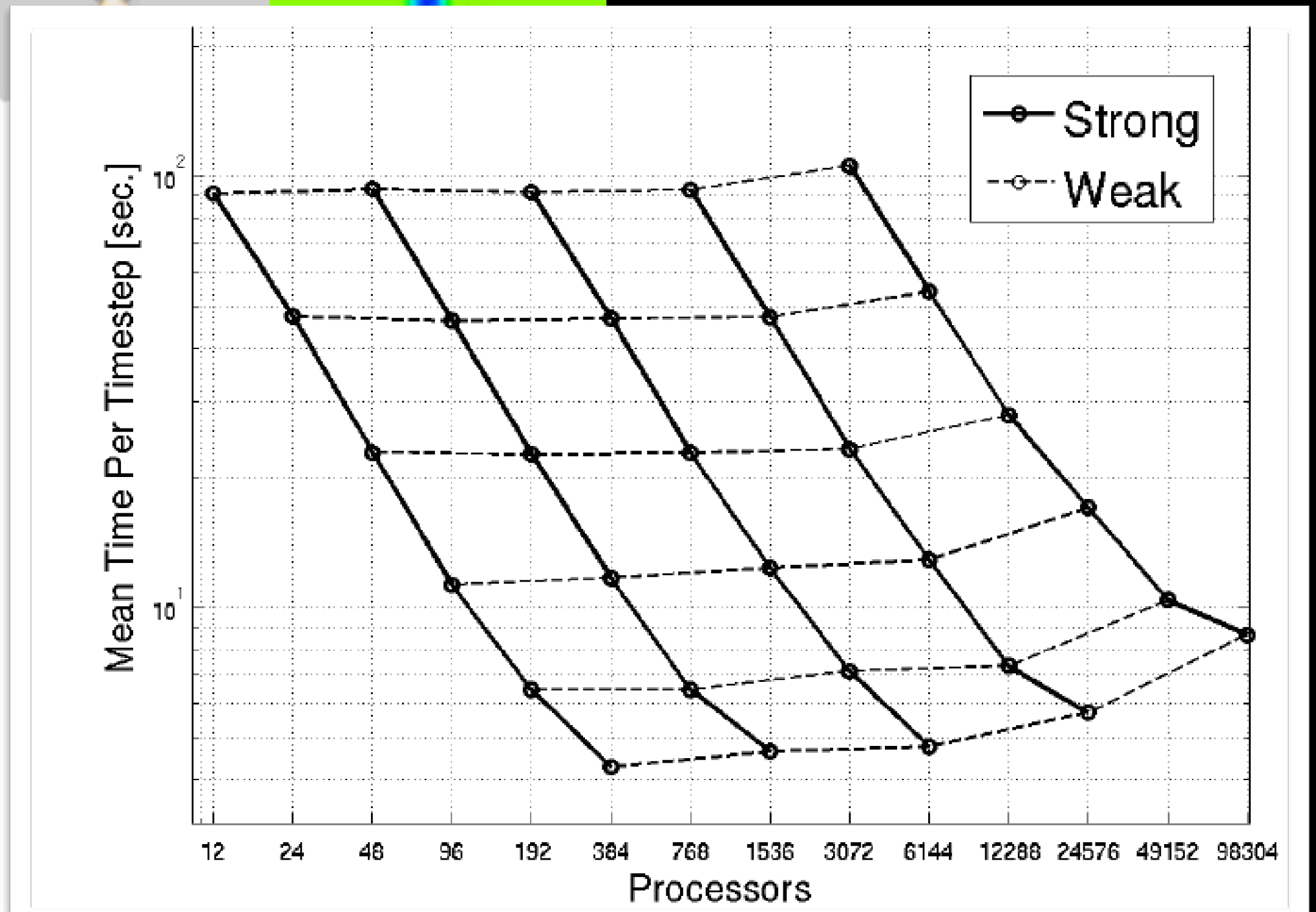


RANS-ebu

- burner performance (oxy-coal w recycled flue gas)
- heat transfer in boiler

Accelerate Deployment: HPC (oxy-coal)





Accelerate Deployment: HPC (oxy-coal)

Demonstration

Burner & Boiler
350 MWe Design
LES & V/UQ

Task 9

Alstom BSF
15 MWt

Task 9

BYU
sifier
-fired)

Task 5

L1500
1.5MWt

Task 3

OFC
100KW
(ignition)

Task 9

Particle-scale Models

Particle Reactions
Sandia (Shaddix)
laminar oxy-coal

Task 5

Non-Reacting Gas & Coal Jets
(Purdue)

Task 3

UQ - Predictive Validation (V/UQ)

"theories are instruments of prediction. From one set of observable data, theories form a bridge over which the investigator can pass to another set of observable data." (Ernst Mach)

$$\beta_i \geq x_i \geq \alpha_i, \quad \text{for } i = 1, ..., n$$

$$u_e \geq [y_m(\mathbf{x}) - y_e] \geq l_e, \quad \text{for each } e \in \mathcal{E}$$

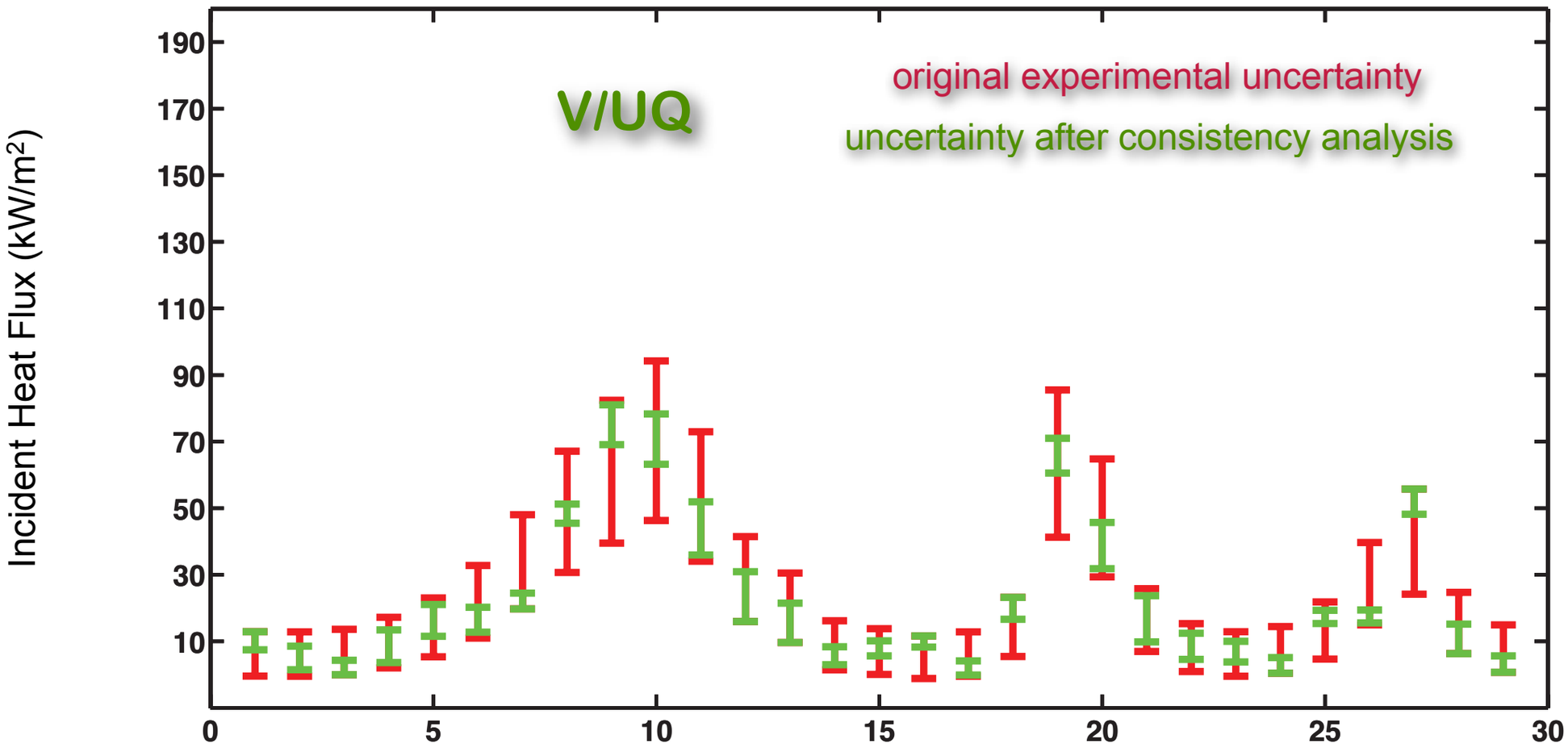
- **models**
- **numerics**
- **scenarios**

Bayesian probability:

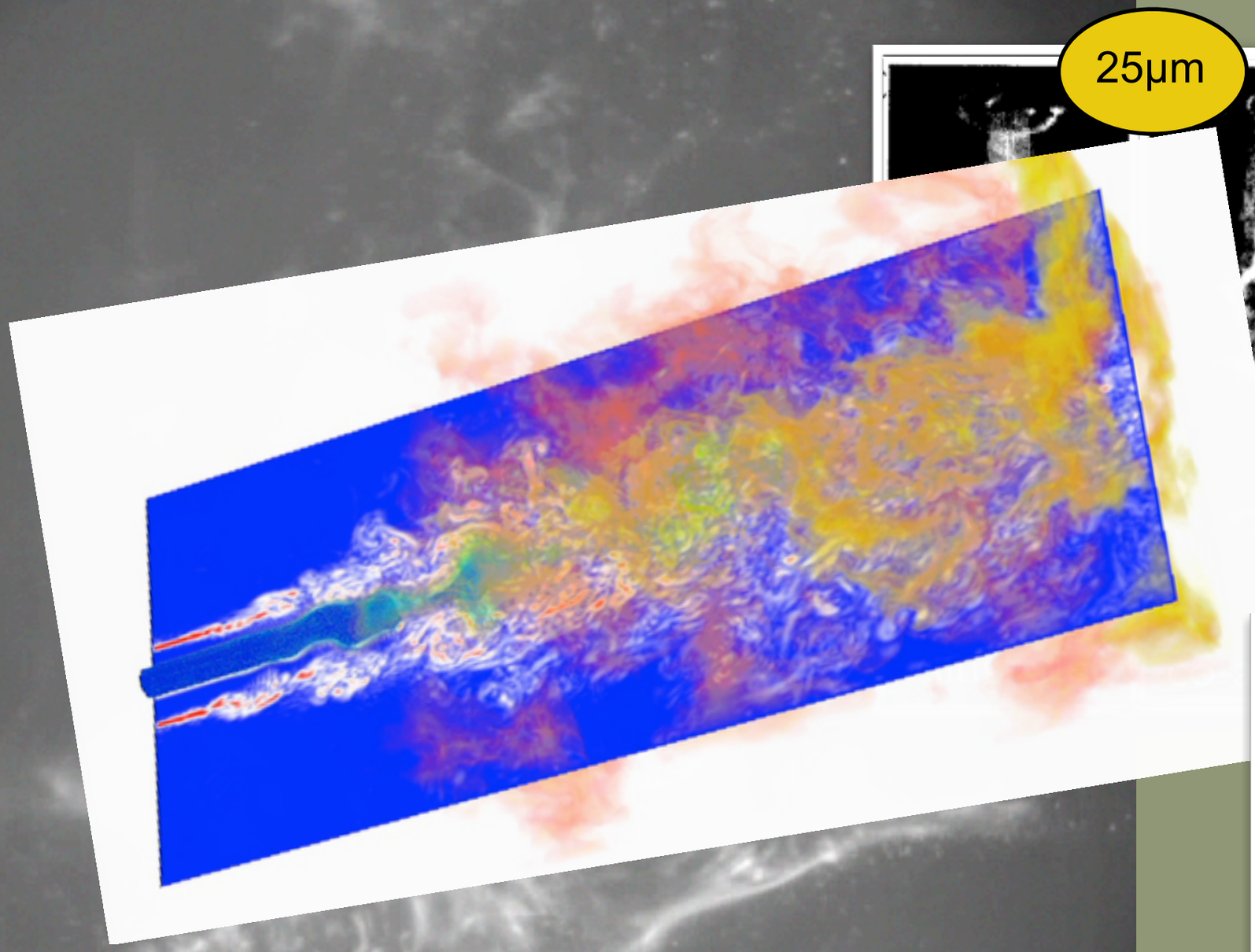
- *probability as "a measure of a state of knowledge"*
- *enables reasoning with uncertain statements*
- *specifies some prior probability which is updated in light of new data*

V/UQ: heat flux from large experiment & simulation

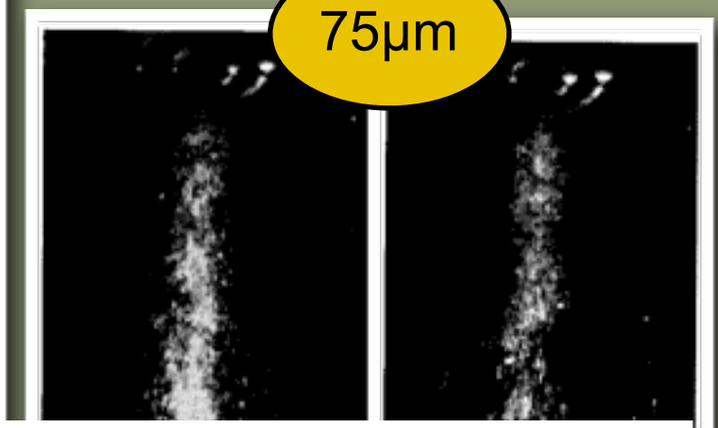
$$u_e \geq [y_m(\mathbf{x}) - y_e] \geq l_e,$$



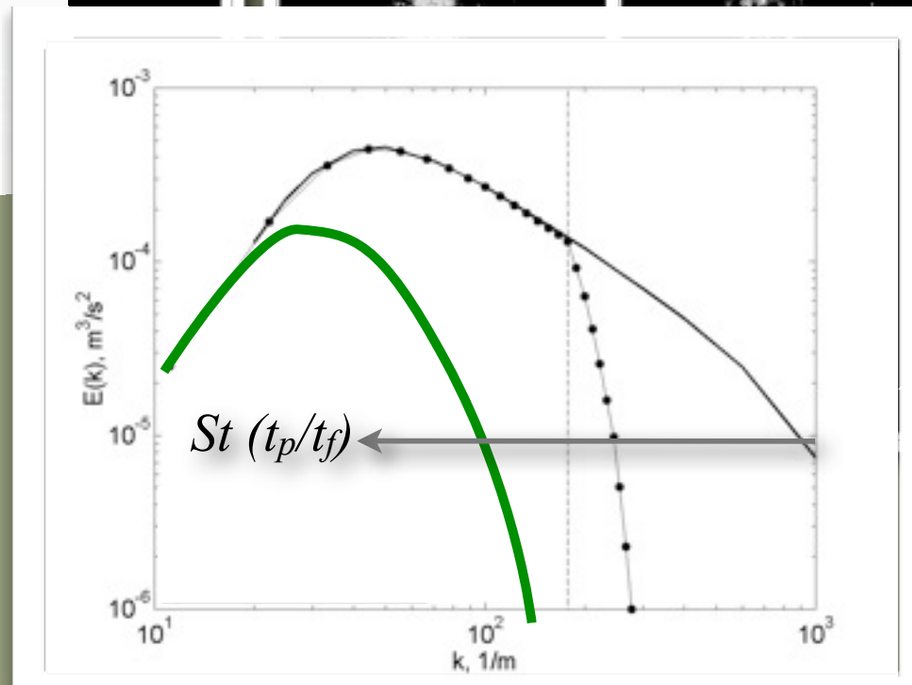
Stokes Number Effects: clustering & segregation



oxy-coal, near burner (T. Ring, UofU)

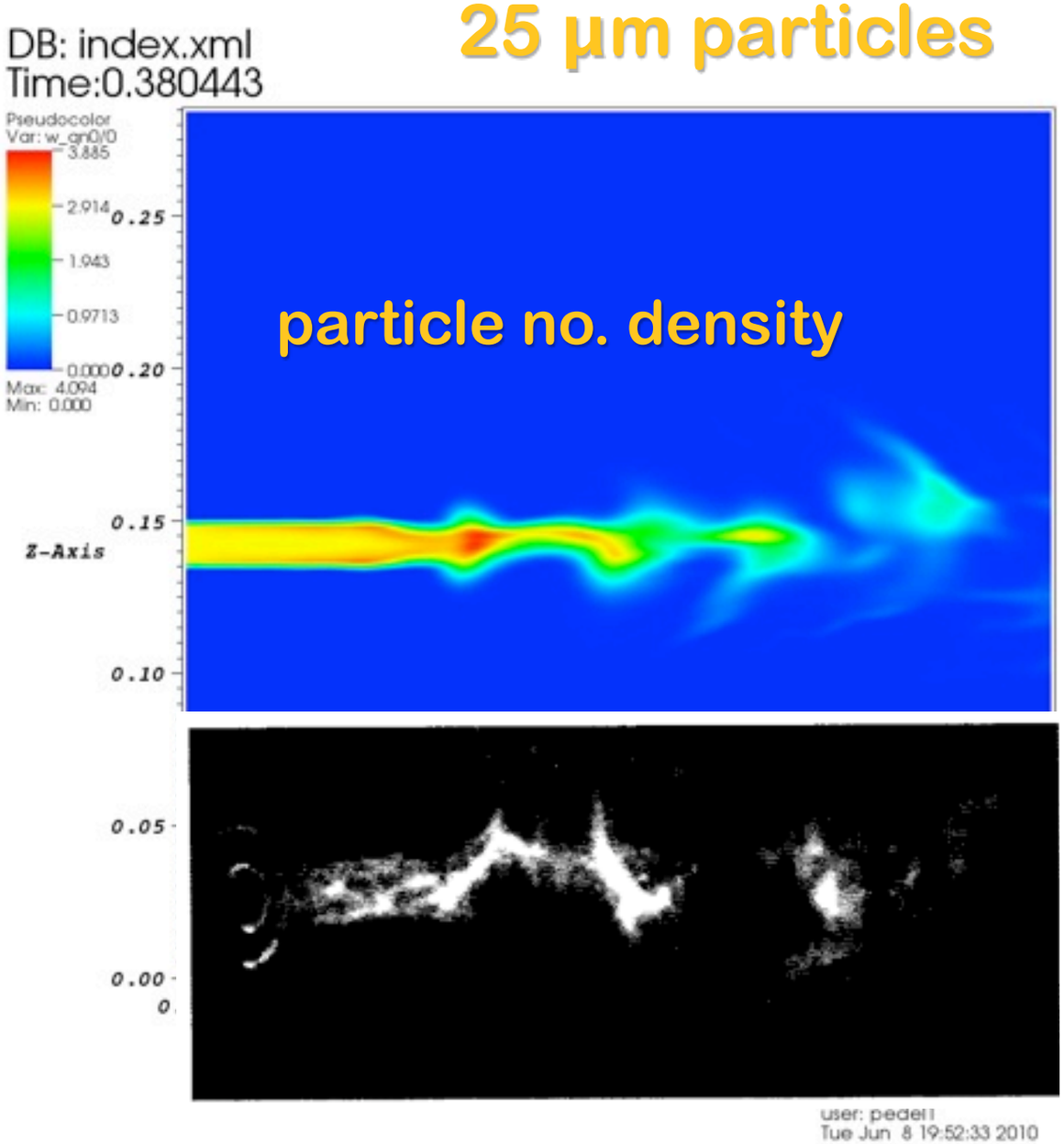


particle-laden jet (S.G. Budilarto, Purdue)

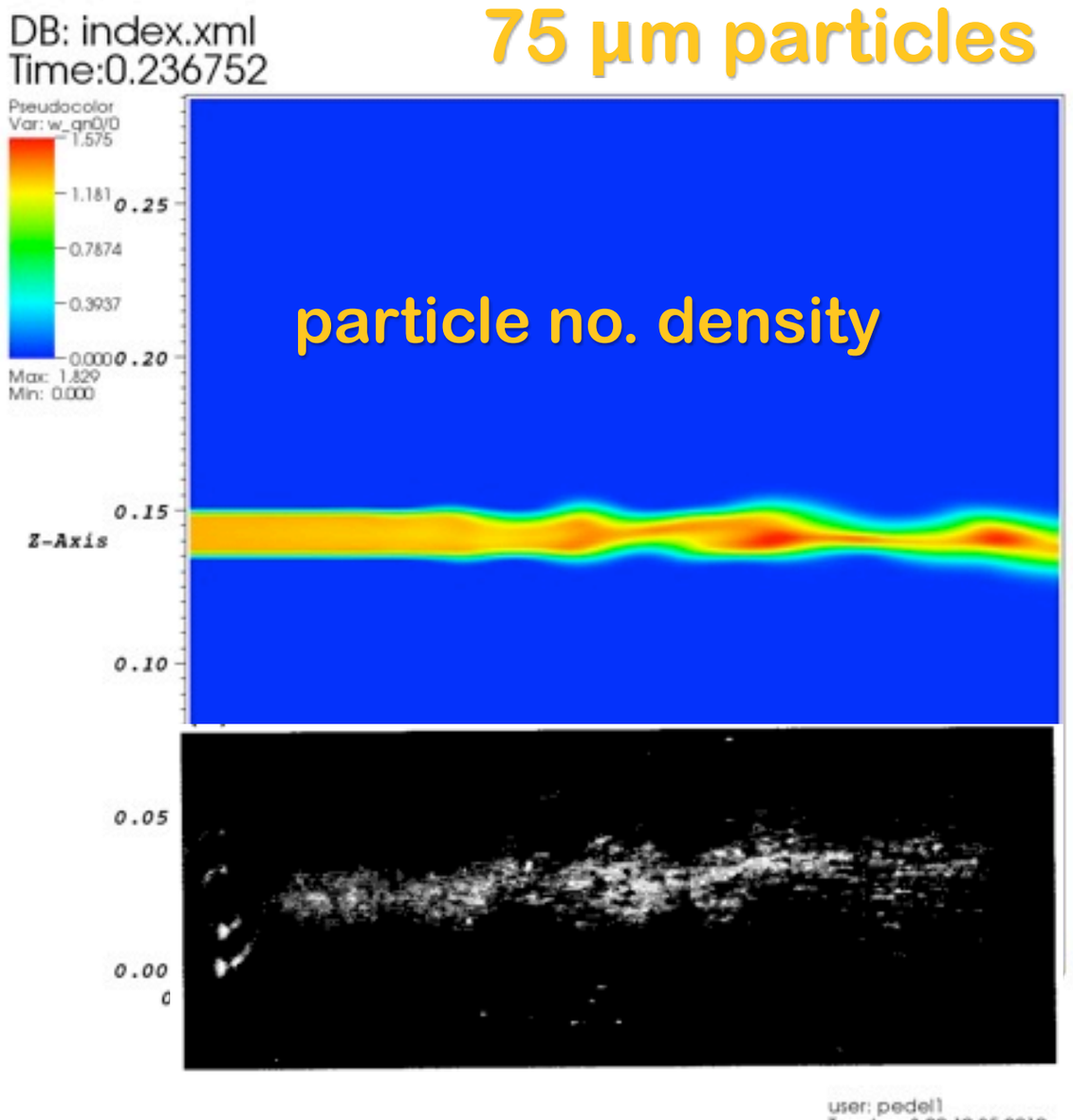


V/UQ observations: Non-Reacting Two-Phase Jet ($velocity_{secondary}$ / $velocity_{primary}$ = 1.5)

25 µm particles



75 µm particles



V/UQ observations: Non-Reacting Two-Phase Jet (velocity$_{secondary}$ / velocity$_{primary}$ = 1.5)

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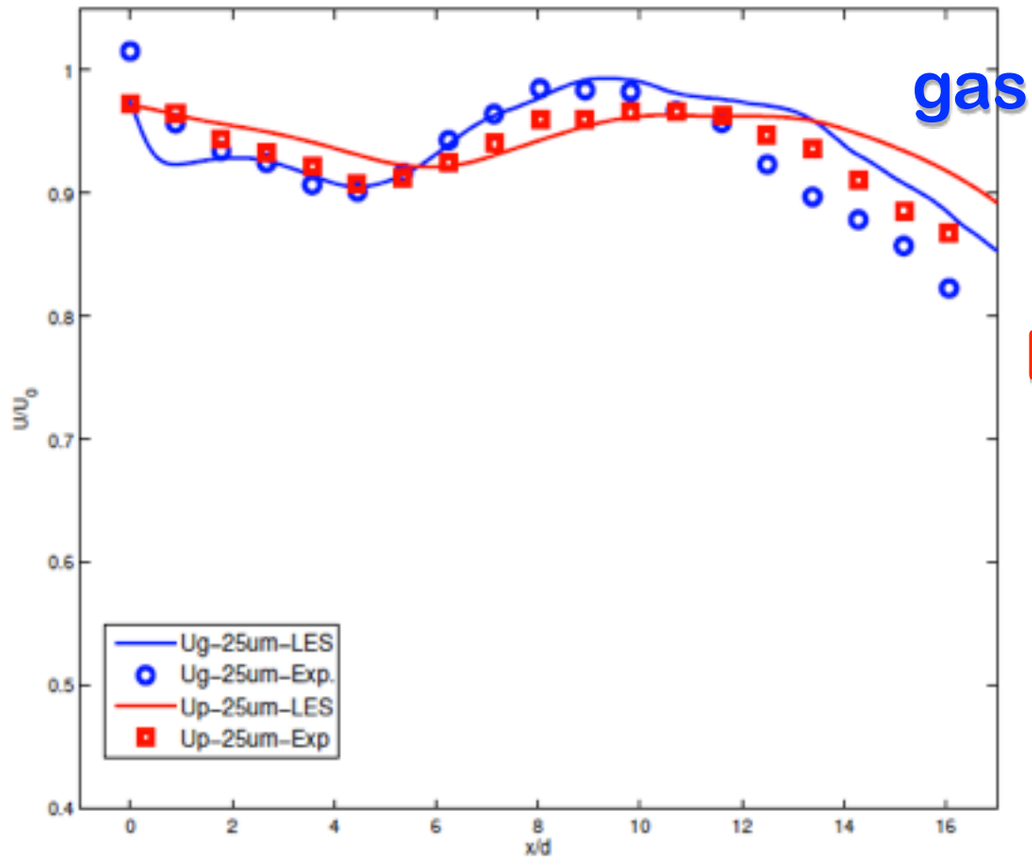
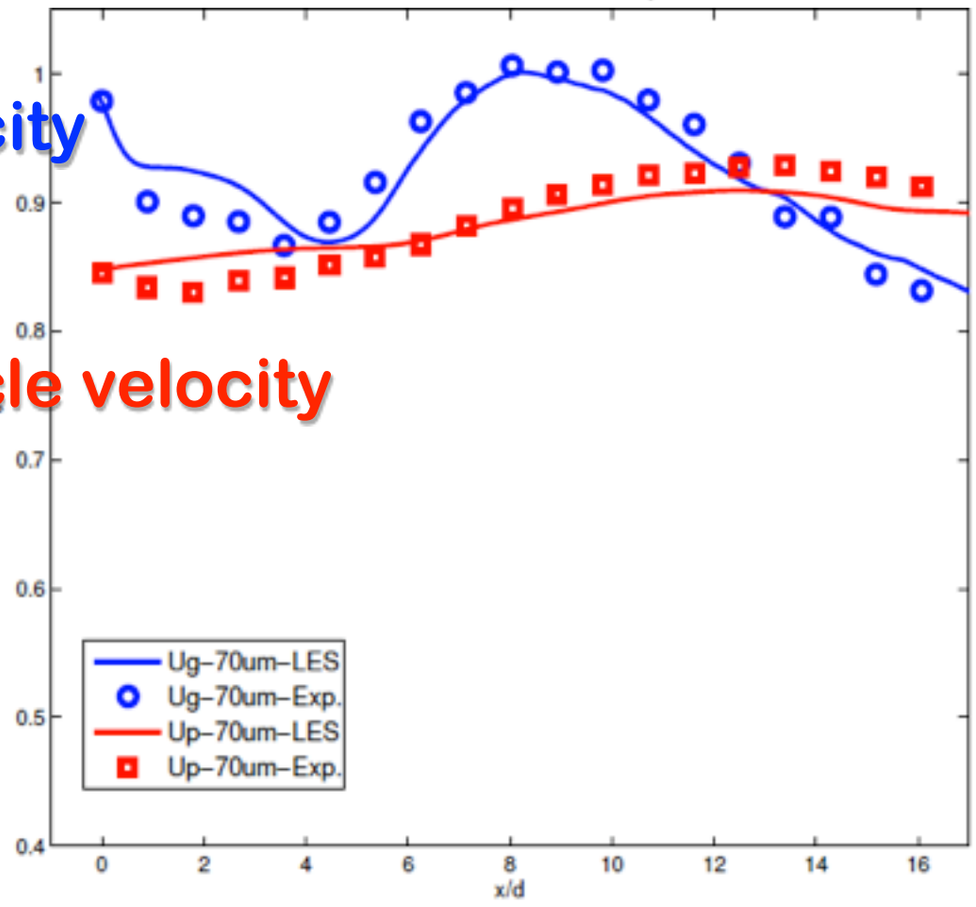


(e) VR = 1.5

gas velocity

particle velocity

75 µm particles

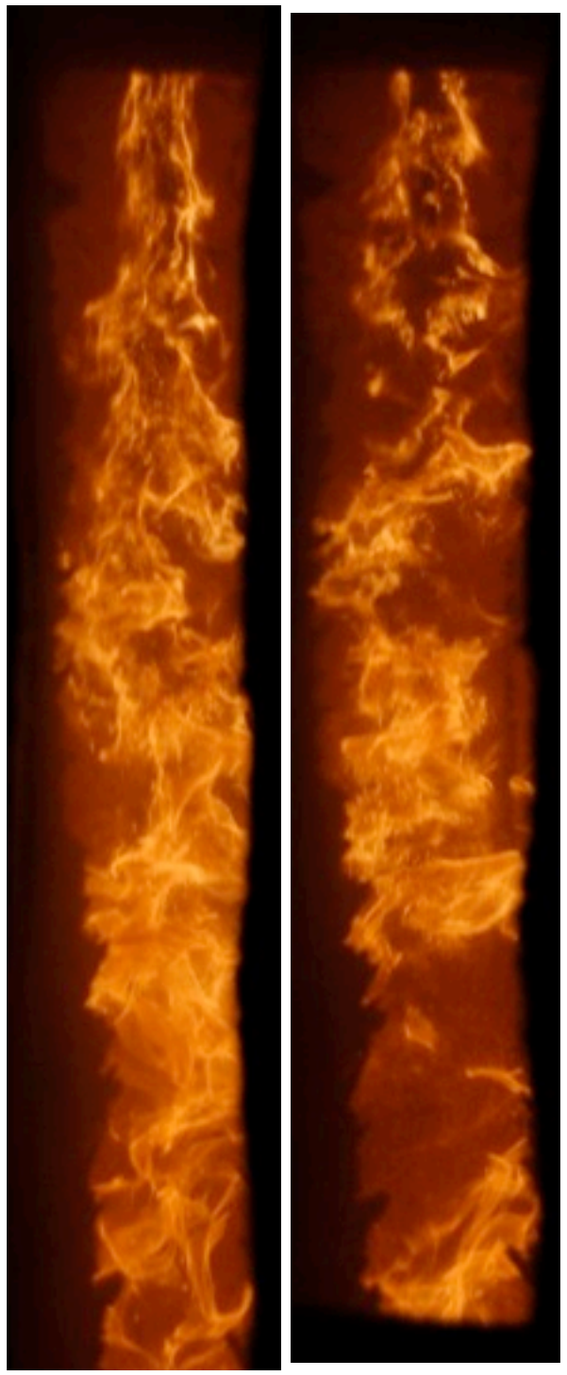


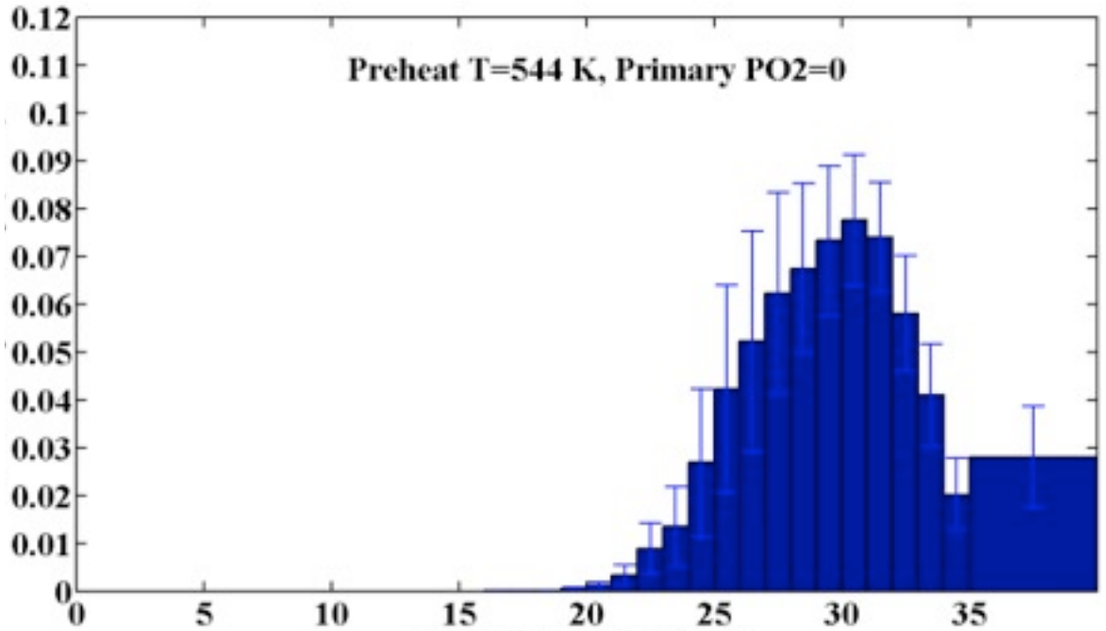
(f) VR = 1.5

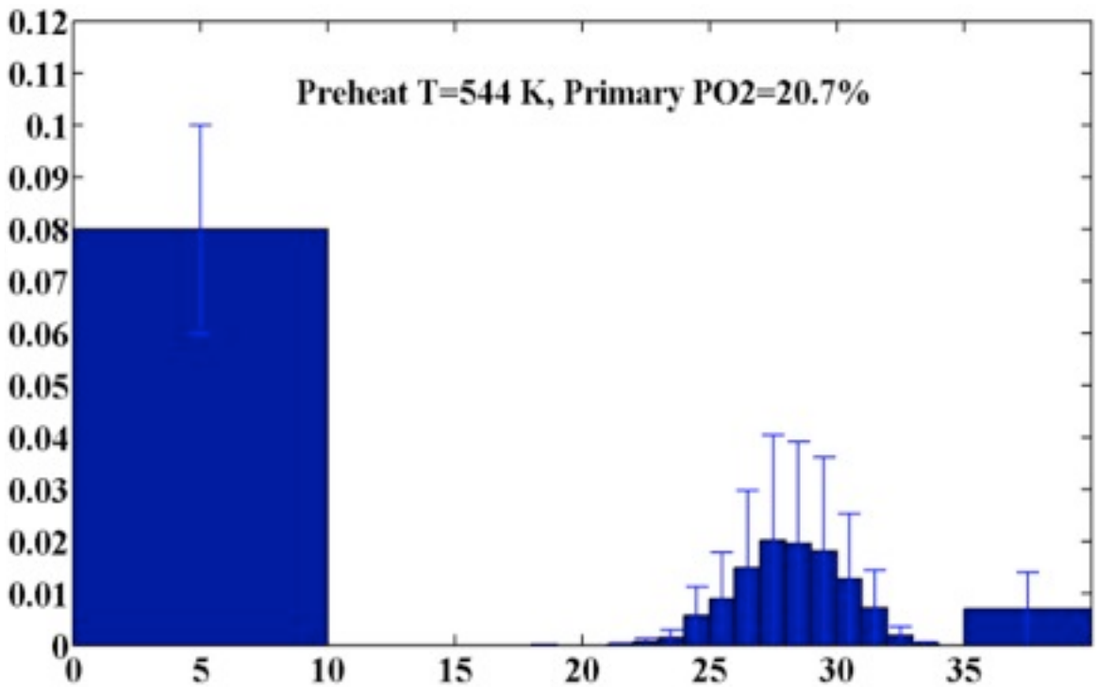
$[O_2]_{primary}$ effect: burner stability

$P_{O2(primary)} = 0\%$

$P_{O2(primary)} = 21\%$





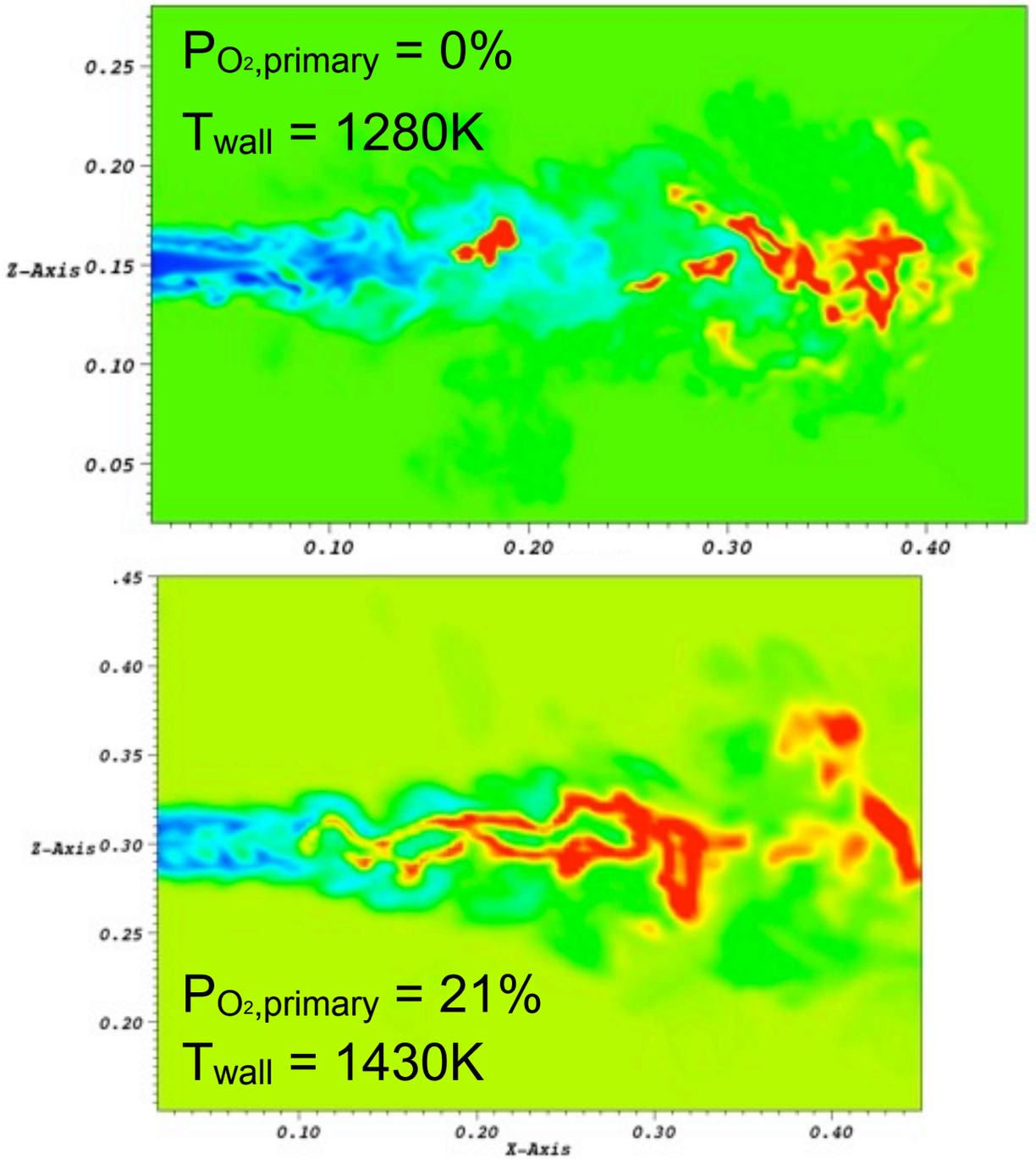


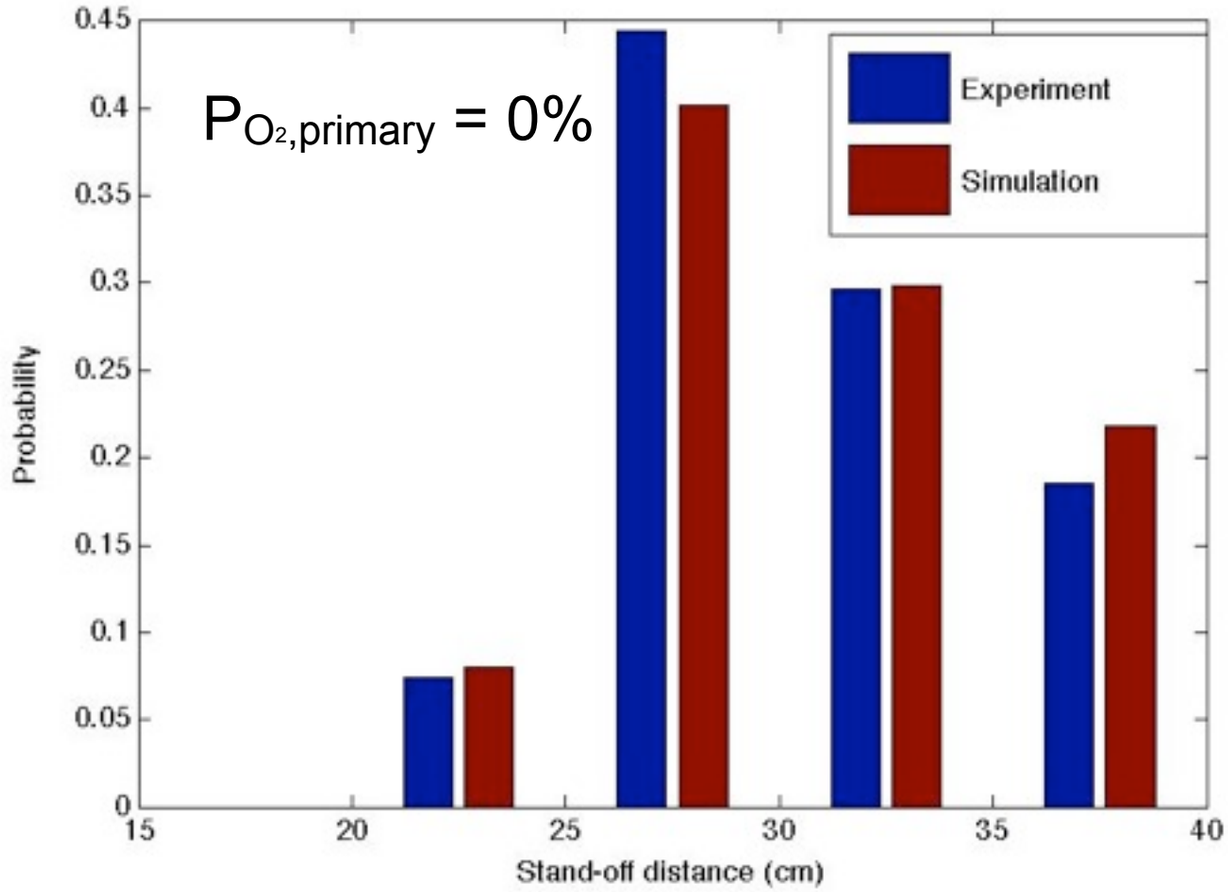
V/UQ observations: predictivity & sensitivity

P_{O_2} primary	Wall temperature (K)	Prior (expt) mean stand-off distance	Posterior mean stand-off distance
0% +/- 1%	1283 +/- 150 K (bias error)	30 +/- 2.5 cm	31 +/- 1.0 cm
20.9% +/- 1%	1283 +/- 150 K (bias error)	12 +/- 2.5 cm	10 +/- 0.5 cm

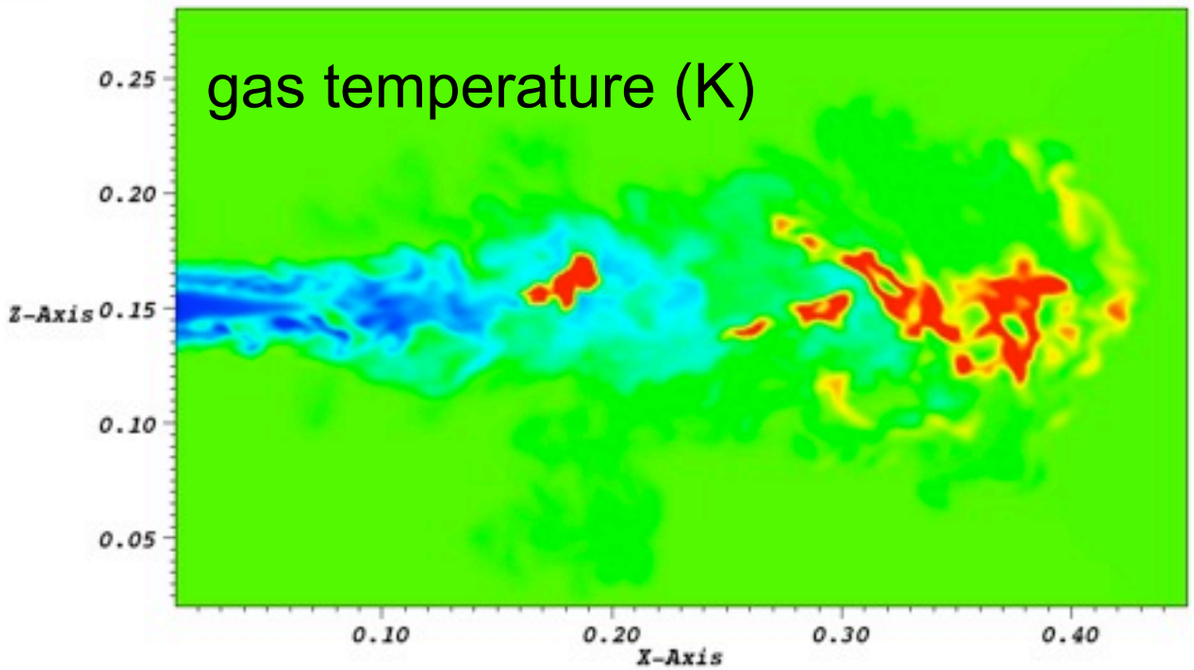
- experiments: high sensitivity to P_{O_2} in the primary
- V/UQ: high sensitivity to wall temperature (preliminary)

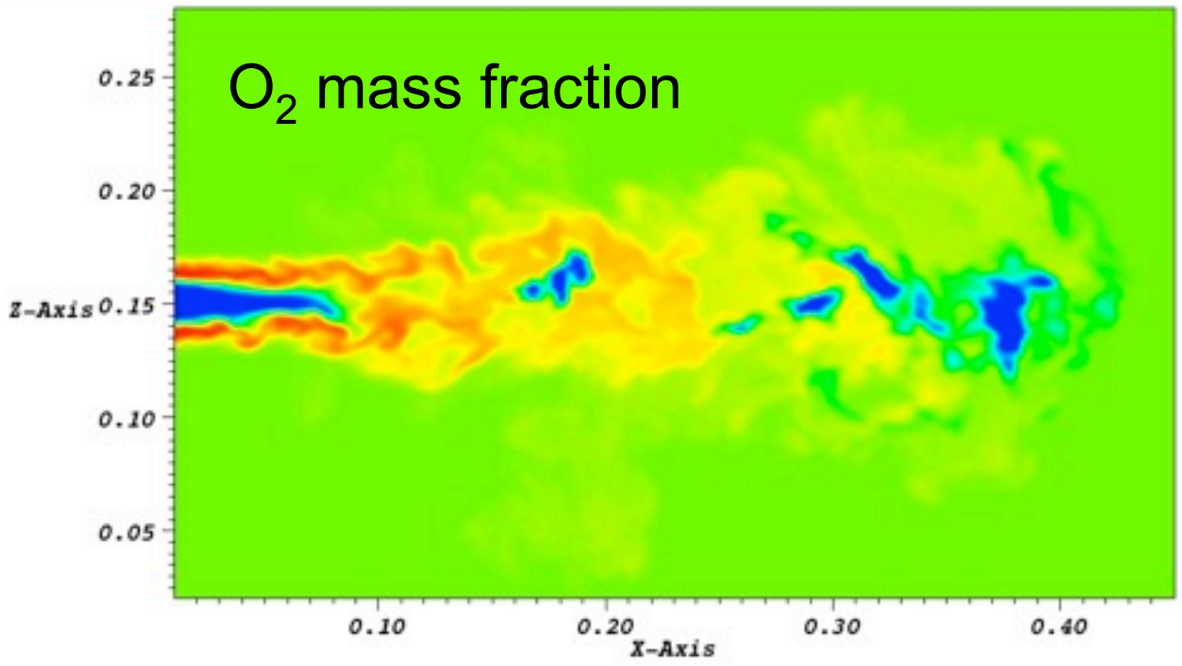
V/UQ observations: stand-off

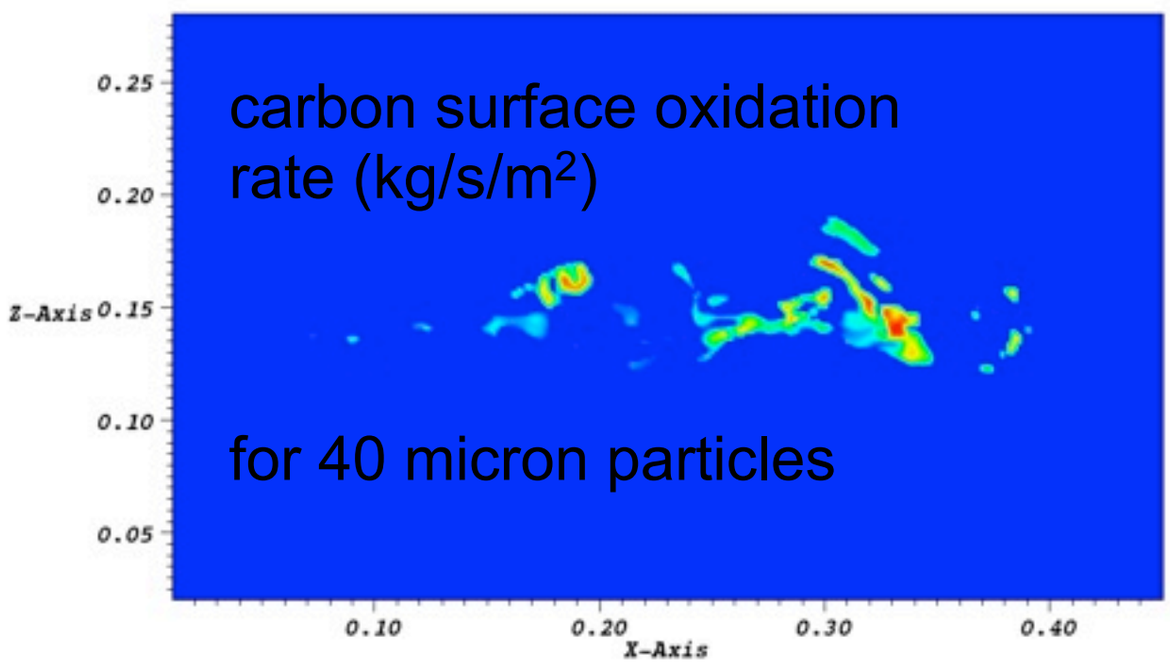




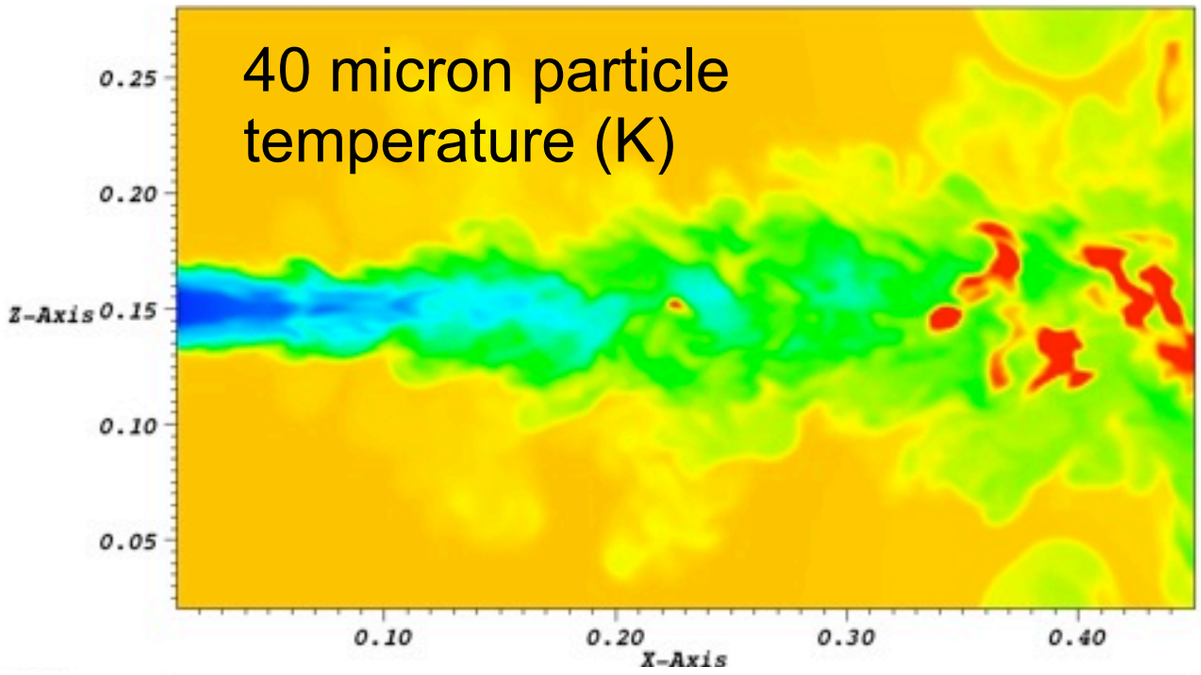
V/UQ observations: surface oxidation ($P_{O_2,primary} = 0$)





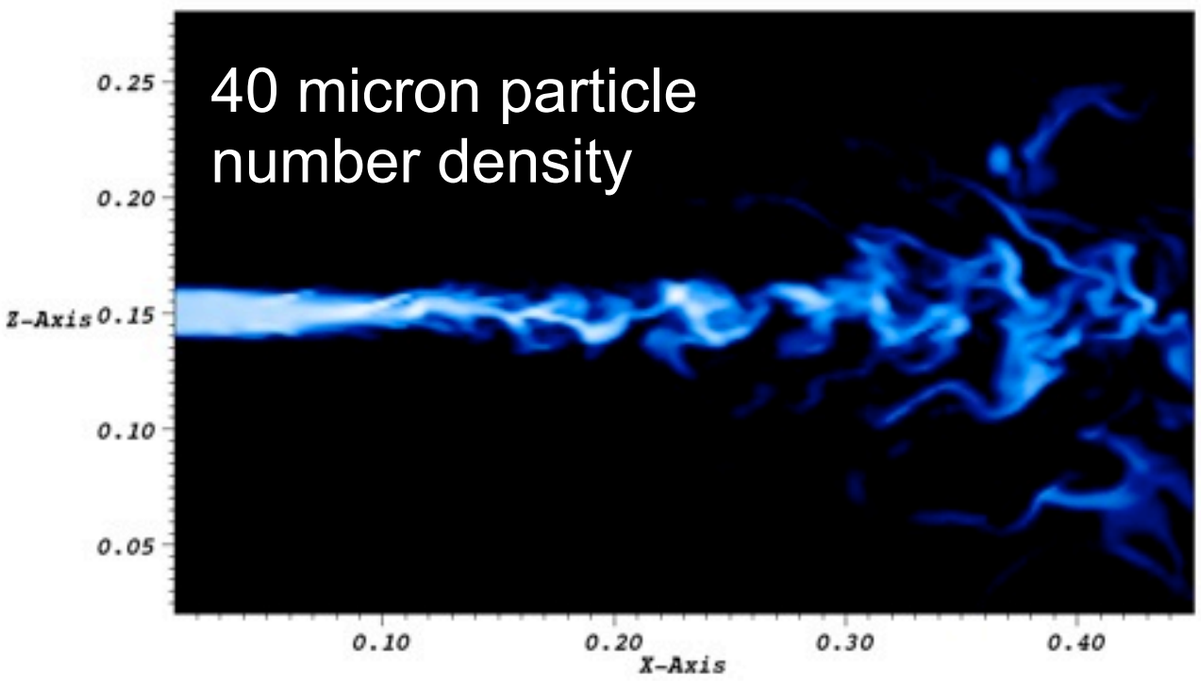


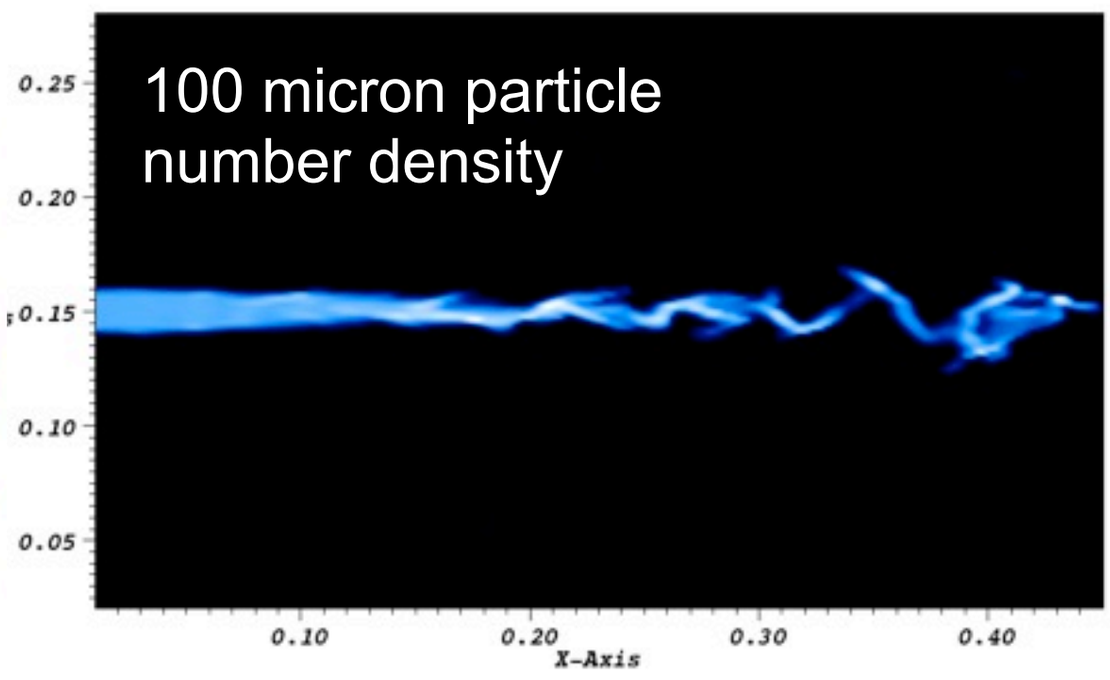
V/UQ observations: ignition mechanism



- **Ignition associated with dynamic clusters of small particles**

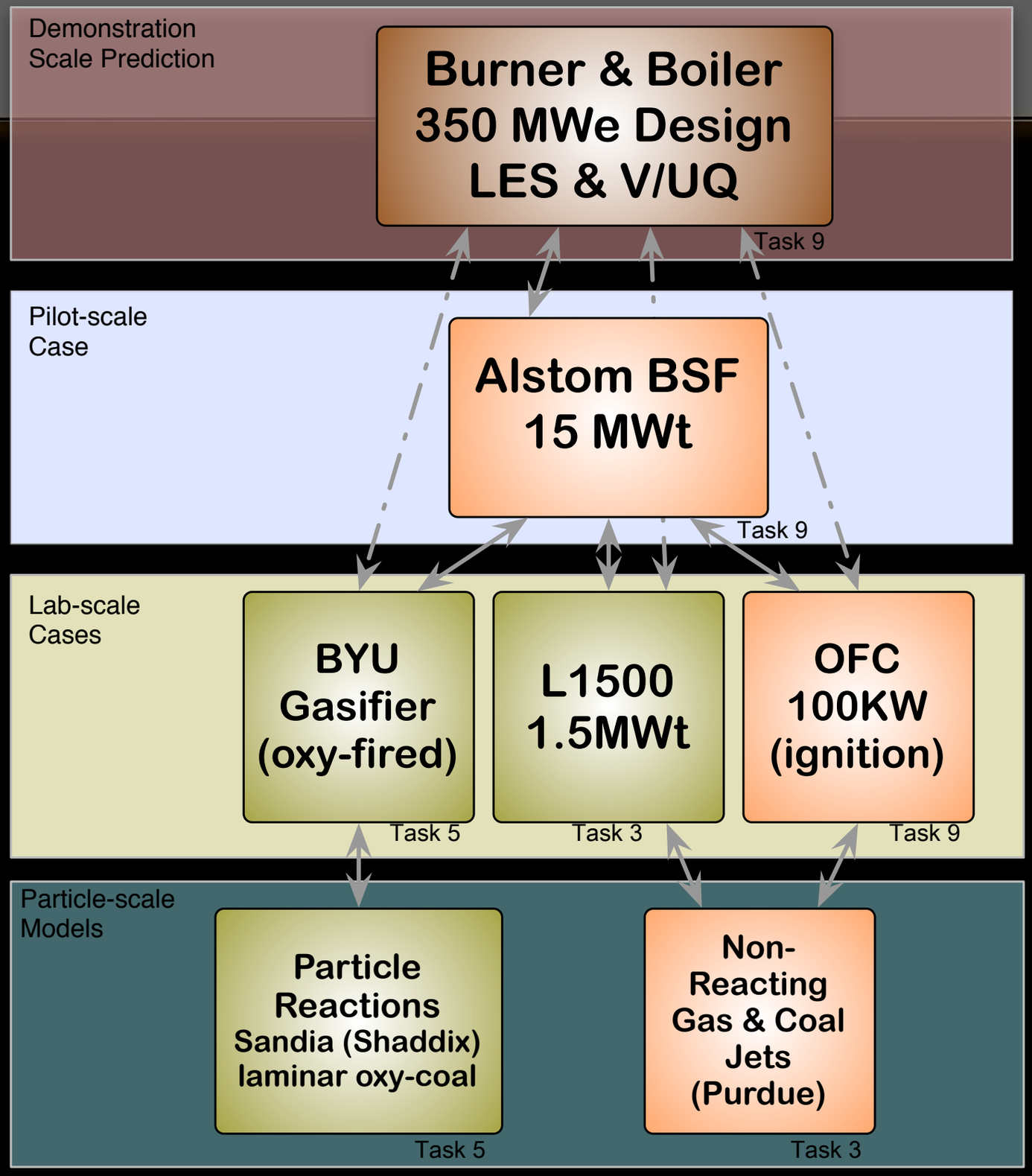
- **In the near burner region, particles heated by radiation from the walls and cool down by convection with the gas**





Path Forward:

- Predictivity through formal Validation/Uncertainty Quantification:
  - by integrated use of simulation and experiments can we facilitate scale up, reduce deployment time, and reduce risk, thus lowering deployment cost ?
  - improve understanding of flame physics under oxy-coal combustion conditions
- Support DOE's Carbon Capture Simulation Initiative (CCSI)



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